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Studying the Resonance Processes in the Surface Layers of Friction Pairs with Lubrication by Means of Molecular Dynamics

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Abstract

The article investigates the resonances of diffusion processes using molecular dynamics method (MD) for heat-resistant steel carbonitriding. For this purpose, three types of resonances processes are used, different in terms of influence of thermal shock (TS) in the surface layers of heat-resistant steel with carbonitriding coating. The first type is nonlinear (cubic) resonance based on the frequencies of atomic fluctuations, ω_0 in crystal lattice α-*Fe* and frequency under force of TS, ω. The second type is associated with resonance harmonics $\omega(i)$ force of TS and spectrum of atomic fluctuations in the lattice. The third type is related to the damping law of attenuation resonance processes in the depth of the surface. The article explores the first type of resonance processes. The result of resonance process conduction in the surface layer occurring to phase structural transformation reduces the formation of secondary structures, which determine the performance properties of the friction pairs.

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Keywords: the resonance mechanism of diffusion; the method of molecular dynamics; thermal shock; secondary structures; structural phase transitions; sliding friction with lubrication.

1. Introduction

During friction, in the surface layers of friction pairs occurs structural-phase transformations leading to the formation of secondary structures which determine the operational properties of friction pairs such as the propensity to grasp, associated with a sharp increase of the local friction factors [1]. The formation of secondary structure is associated with diffusion and diffusion-free (polymorphic) processes in the surface layers. A significant increase in the diffusion coefficient (D = 10^{-5} - 10^{-8} m^2/s) was established experimentally. This phenomenon is determined:

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firstly, by the morphology of the frictional surfaces in the form of sub- and micro-roughness during friction process to the appearance of the pulsating thermal processes (thermal cycling) [2]; secondly, as a result of thermal cycling occurring to thermal shocks (TS) and the related increase in pressure P at the surface zone [3]. Thus, it is in this context, there is a necessity for research into the mechanisms of diffusion, as the widely used diffusion mechanisms (vacancy, exchange, etc.) could not be exploited to explain the sharp increase in the diffusion coefficients.

Recently, methods of molecular dynamics (MD) have been used for the study of diffusion processes which allow to study these processes through simulation, which has its own characteristics. If during simulation the nuclear lattice and electrons are partially neglected and only the volumetric phenomena (the continuum) is considered, then in the simulation of diffusion processes it is preferable to consider the processes at the level of the crystal lattice. Since conclusions about the mechanisms of diffusion should be done on the basis of the energy estimation and the controlling process, it is necessary to set the binding energy between atoms in the form of potentials of pair interactions (PPI). The presence of PPI raises the possibility of formation of a crystallite with a given set of properties with the given number of atoms N (usually $N \leq 10^5$). Therefore, the oscillatory processes are considered in the simulation since the wave processes occur in the metal when $N \geq 10^6$ [4].

In the works [5, 6] is presented the results of simulations MMD about the movement process of atoms under the influence of TS in the surface zone of complex alloy heat resistant 25Kh3M3NBTsA. The analysis of trajectories of movements of atoms has allowed to define the diffusion mechanism as cooperative (relay) with diffusion coefficients $D = 10^{-6}$ - 10^{-8} м^2/s. However, to explain the higher experimental diffusion coefficients in the order of $D = 10^{-5}$ м^2/s, this mechanism is not possible. Preliminary estimates showed that another mechanism may occur under the influence of TS defined as resonance. This assumption is based on the possibility of matching the frequency (ω_0), vibrations of the atoms in the crystal lattice vibration frequencies (ω), and external force (TS).

Experiments have revealed the presence of crystals in the zones with abnormally high amplitudes of the vibrations of the atoms without external influence. The theoretical justification of this phenomenon was given by M. Born [7]. The presence of impurities and defects in the crystal affects the spectrum of vibrations of atoms due to the appearance of oscillations, called localized modes. For sufficiently large distortions of the lattice can occur in resonant modes, resulting in micro-volume resonances. In [8], where they studied lattices with strong anharmonic state and took into account collective phenomena in phonon subsystem, it is established that as a result of nonlinear resonance and synchronization occurs the phonon frequencies. These processes lead to structural instability of the lattice, martensitic transformations and melting.

2. Formulation of problem

Resonant processes during friction are fast ($\tau \approx 10^{-12}$ s). In this regard, the modelling of these processes is obviously preferable. In the simulation the resonance is defined as a sharp increase in the amplitudes of the forced vibrations of N atoms, arranged in a set of lattices representing the imaginary crystallite. The atoms undergo thermal vibrations with frequencies ω_0 and subjected to external periodic effects (TS) with the frequency ω. According to Born-Lederman theory the frequency distribution of fluctuations of the real metal, presented in the form of a large lattice of N atoms approximately coincides with the distribution of imaginary frequencies of the lattice with cyclic boundary conditions [7]. In turn, an imaginary system of N atoms is completely equivalent to a chain of simple harmonic oscillators with corresponding frequencies ω_0^i. If this chain link PPI, in the language of the theory of vibrations the motion of atoms in the chain is defined as the movement of the oscillators in the field, given PPI [9]. In the absence of external effects (TS) such a system is mathematically described as autonomous. Since the crystal lattice has PPI rigidity, its fluctuations are dissipative. If the decomposition of the PPI members consider the 3rd order, i.e. thermal anharmonicity, then, first of all, the system will be nonlinear (cubic), and, secondly, there are the dispersion of the frequency (spectrum), as the anharmonic members provide a link between normal lattice vibrations. If we consider the anharmonic terms, the terms of higher order play essentially the role of viscous medium, dissipating the energy dispersion of the oscillators. In the presence of TS system becomes a non-autonomous cubic nonlinear dissipation and dispersion. The mathematical description of such a system is given by [9]:

$$\ddot{x} + \omega_0^2 x = -2\gamma\dot{x} + \beta x^3 + f\cos(\omega + \varphi), \tag{1}$$

where left side of equation is atomic thermal fluctuations with frequencies ω_0, right side equations is parameters reflection exposure of TS.

Atomic fluctuations ω_0 in chaotic. To spot main frequency ω_0, based on research of M. Born [7], the formula told about characteristic of its own limit. Correctly, atomic chaotic fluctuations of atoms notion "spectral fluctuations". To analysis description of spectral (spectral dispersion) with classical method significant difficulties. Simultaneously, method of quantum is used to determine questions of spectral fluctuations of atoms. Particularly, to describe spectral fluctuations used function of thickness fluctuations of atoms (density of phonon spectral). Lately, for this purpose usually used discrete conversion of Hartley [10], eases to apply in program XMD.

Additional note, very important to analyze pair potentials using EAM method, to compute pair potentials, already in work [11].

3. Results and discussion

The main idea of this research was to compare the result of analysis of non linear amplitude resonance A, with different frequency combinations ω_0 and ω_1 and parameter a in crystal lattice. On assuming $A > a$, the atoms break loose from lattice, which actually initiates the process of diffusion. If $A \leq a$, then there will be a resonance oscillations without diffusion (it's called increasing activity of atoms). However, the lattice will be in tension, since relaxation takes place after atoms leaves the lattice. Therefore, in this situation process of diffusion begin after resonance act $(n = a/A)$.

For getting these parameters of resonance, represented in equation (1) as follows:

$$\ddot{x} + 2\gamma\dot{x} + \omega_0 x - \beta x^3 = f\cos(\omega + \varphi). \tag{2}$$

Equation (2) represents the nonlinear differential equations without any option of obtaining analytic solution. At work [9], considering the differences in solving methods for particular problems, it represents the other one of them: the method of slowly varying amplitudes. Suggested solution of the equation (2) as a resonance curve of the equation:

$$(\gamma A)^2 + A^2\left(\delta\frac{3\beta A^2}{8\omega_0}\right)^2 = \frac{f^2}{4\omega_0^2}, \tag{3}$$

where $\delta = \omega$-ω_0 – the detuning frequencies.

This equation implicitly defines sought frequency of the resonant oscillations as a function of the amplitude and frequency of the driving force. To obtain an explicit result of the equation (3), transformed more convenient analysis form to minimize the number of variables and parameters. To be specific, we assume that the parameter β of nonlinearity (anharmonism) adverse.

Introduce the following notation.

Non-dimensional parameter characterizing the intensity of external influence:

$$Q = \frac{3\beta f^2}{32\gamma 3\omega_0^3}. \tag{4}$$

Non-dimensional parameter characterizing the intensity of the forced oscillations:

$$X = \frac{3}{8}\frac{\beta A^2}{\gamma\omega_0}. \tag{5}$$

A dimensionless the detuning frequencies:

$$\Delta = \frac{\delta}{\gamma} = \frac{\omega - \omega_0}{\gamma}. \tag{6}$$

As a result, the equation (3) takes the form:

$$X = \frac{Q}{(X + \Delta)^2 + 1}. \tag{7}$$

Using these results to analyze resonance processes for complex alloy heat resistant 25Kh3M3NBTsA, overpass the thermo-chemical treatment – low-temperature carbonitrided process (carbonitriding). The primary element in the chemical composition is *α-Fe*, which has body-centered cubic lattice (BBC). We calculate the value of the required parameters coefficients of the equation (2). Mass of atom *Fe, m* = $0.927 \cdot 10^{-25}$ *N*·s^2/м, atomic radius *r* = $1.26 \cdot 10^{-10}$ *N*, Parameter lattice *a* = $2.87 \cdot 10^{-10}$ м. The relative force of the external influence is defined as:

$$f = \frac{PS}{m} = P\frac{\pi r^2}{m} = 5.378 \cdot 10^5 \cdot P. \tag{8}$$

The pressure *P* is determined by TS friction temperature at sub roughness [3]. Parameter *f* given in Table 1.

Table 1. Parameter *f* and Thermal Shock (TS) frequencies according to the temperature.

T, ^{0}C	200	300	400	500	600	700
P, GPa	6.40	8.1	10.8	14.7	16.7	19.2
$f \cdot 10^{-15}$, м/s^2	3.49	4.44	5.92	7.4	8.88	10.36
$a \cdot 10^6$, м/s^2	10.49	9.2	8.3	7.12	6.06	4.95
$u_f^{(1)} \cdot 10^{-12}$, 1/s	2.96	3.2	3.48	4.32	5.54	6.8
$u_f^{(2)} \cdot 10^{-12}$, 1/s	1.48	1.6	1.74	2.16	2.77	3.4
$u_f^{(3)} \cdot 10^{-12}$, 1/s	0.74	0.8	0.87	1.08	1.39	1.7

Base frequency is determined by the external influence of the dependence [12]:

$$\omega_1 = V_{so}^2 / a_0, \tag{9}$$

where $V_{so} = 5{,}8 \cdot 10^3$ м/s – velocity of sound in the crystal; a_0 – the thermal coefficient of the crystal.

The low-order of Harmonic fluctuation is determined by a discrete wavelet transform (DWT). As the main been used Morley wavelet with the central frequency *Fr* = 0.8125 Hz [13]. The Wavelet Toolbox is a collection of functions built on the MATLAB Technical Computing Environment [14]. It provides tools for the analysis and synthesis of signals and images using wavelets and wavelet packets within the framework of MATLAB in form:

$$f = 1.48 \cdot 10^{13}(T_c - T_0). \tag{10}$$

The program determines the center frequency of the first decomposition the formula $Fr_1 = \omega_1 = 0.8125N$, where *N* is the general number of counts in 1 second. For subsequent decompositions have central $Fr_2 = \omega_2 = \omega_1/2$, $Fr_3 = \omega_3 = \omega_2/2$, , … harmonic values (up to third) depending on the oscillation frequency temperature T_c as shown in tabl. Graphical interpretation of the discrete harmonic expansion is shown in Fig. 1.

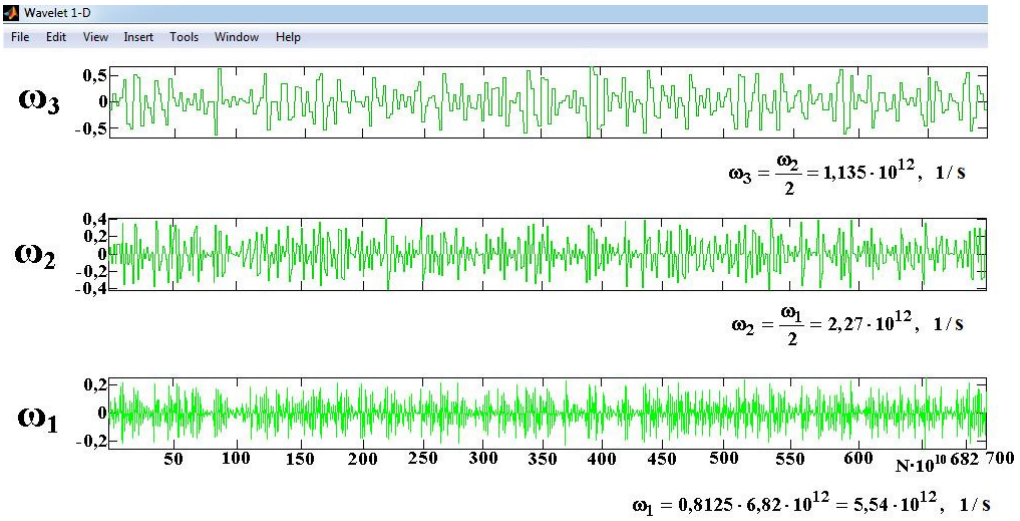

Fig. 1. Discrete decomposition (wavelet transform) ω_1 frequency (a), ω_2 (b), ω_3 (c) external force.

To calculate the density of the phonon spectrum $H(\omega_0)$ discrete Hartley transform (DHT) are used. As with Fourier transform, it can be applied to spectral analysis and various types of signal processing, and it has several advantages, in comparison to the Fourier transform: the calculation of direct and inverse Hartley transforms is carried out by a symmetric formulas, whose form is the same up to a factor *1/N*; direct conversion Hartley provides several of real numbers [9].

To transform into the frequency domain (spectrum receipt) have used autocorrelation function *P(t)* (average dependence of the direction and velocity of the atoms of the module from the initial position of the atoms of the time). Discrete Hartley Transform on this occasion is expressed by the sum of:

$$H(\omega_0) = 1/N \sum_{t=0}^{N-1} P(t) cas(2\pi\omega t), \qquad (11)$$

where $casx = cos\, x + sin\, x$.

The magnitude and direction of atomic oscillations in time for the autocorrelation function were obtained by MD (XMD package source). The simulation was performed with the following parameters crystallite *α-Fe*: the number of atoms – 100; temperature – 400, 500, 600 ^{0}C; a = 2.87 $\dot{A}$; using "clamping temperature method" and recurring boundary conditions. Using approved D. Farkas potential for 20.000 simulation time step steps 10^{-16} c. As a result, these spectral curves have been obtained (Fig. 2).

Graphic implementation discussed resonance diffusion mechanism through XMD software package with regard to the crystallite α-Fe is represented in Fig. 3 a-c.

4. Conclusions

1. Based on the solutions of the nonlinear cubic differential equation describing the oscillations of coupled oscillators under external forces – TS resonance parameters are set, the main of which is the amplitude of the resonance $A = f(T)$.

2. Determine the lower boundary of the beginning of the diffusion process corresponding to condition $A = a$, where a – lattice parameter.

3. As a result of resonant processes occurring in the surface layers of structural and phase transformations it leads to the formation of secondary structures, which determines the performance properties of friction pairs.

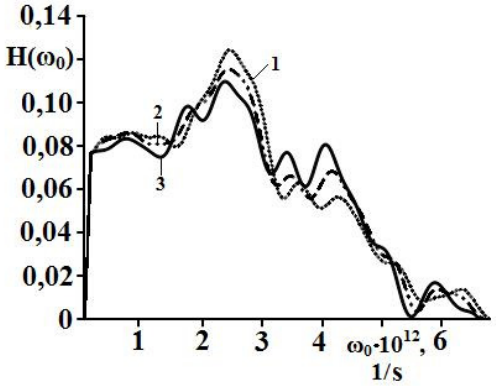

Fig. 2. The dependence of the density of the phonon spectrum *H α-Fe* from the frequency ω_0 of oscillations of atoms at a temperature *T*=400 (1); 500 (2); 600 ^{0}C (3).

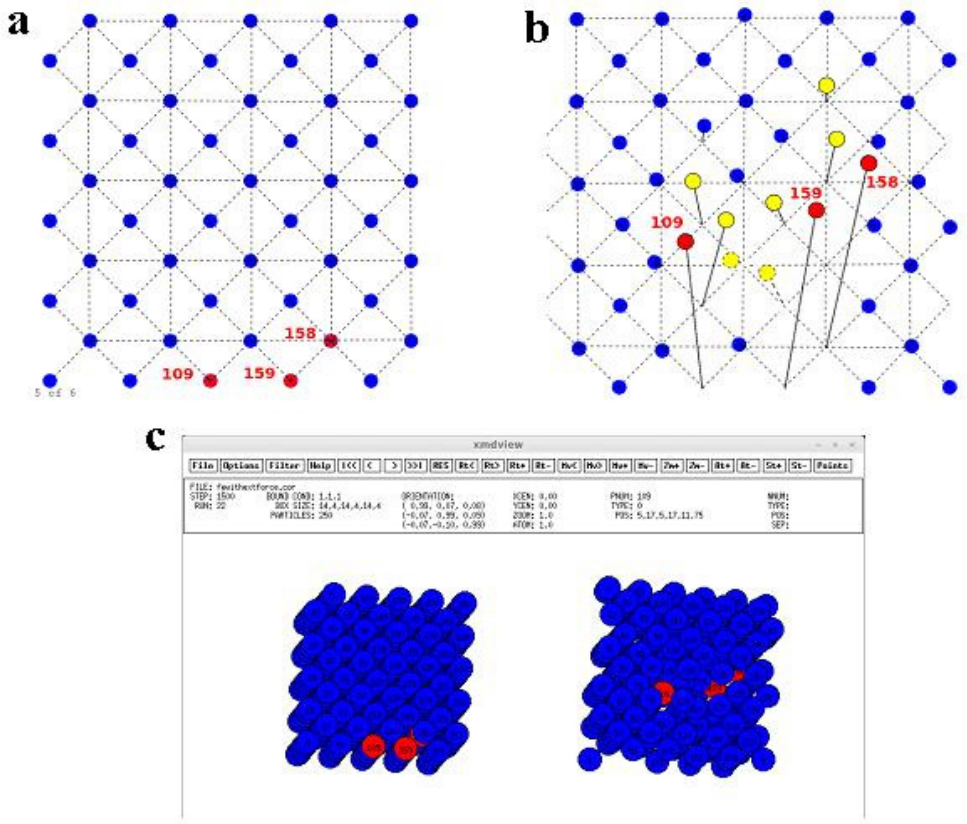

Fig. 3. Crystal *α-Fe* with the number of steps (a) 0; (b) 1500; (c) implementation via XMD software package.

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